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DEGRADATION OF INTERFACE INTEGRITY BETWEEN A HIGH-K DIELECTRIC THIN FILM AND A GATE ELECTRODE DUE TO EXCESS OXYGEN IN THE FILM

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ABSTRACT

In this study, the degradation mechanism of the interface integrity between a hafnium dioxide thin film and a gate electrode thin film was investigated by using quantum chemical molecular dynamics. Effect of point defects such as excessive oxygen and carbon interstitials in the hafnium dioxide films on the formation of the interfacial layer between them was analyzed quantitatively. Though the defect-induced sites caused by oxygen vacancies and carbon interstitials were recovered by additional oxidation after the deposition of the hafnium oxide film, the excessive interstitial oxygen and carbon atoms remained in the film deteriorated the quality of the interface by forming new oxide or carbide of the deposited metal such as tungsten and aluminum. No interfacial layer was observed when a gold thin film was deposited on the hafnium oxide. The estimated changes of the interface structure were confirmed by experiments using synchrotron radiation photoemission spectroscopy. [*Keywords:* High-k Gate Dielectrics, Band Gap, Point Defects, Residual Stress, Hafnium Oxide, Quantum Chemical Molecular Dynamics, Synchrotron-radiation Photoemission Spectroscopy]

INTRODUCTION

Highly reliable gate stack systems using a high-k dielectric thin film such as a hafnium dioxide film and metal tungsten gate are indispensable for the development of sub-50-nm ULSI devices. It is well known, however, that the control of the interfacial crystallographic structure between the dielectric film and a Si substrate or a gate electrode material is one of the critical issues of high performance and highly reliable operation of the devices. [1]-[5] In the new gate stack structures, it is very important to make the sharp interface between the gate oxide and the electrode for assuring the high performance of the stacked MOS structures. This is because that a transition layer between them deteriorates the electronic function of the MOS devices significantly. One of the most troublesome layers is tungsten oxide because it decreases the effective capacitance of the gate oxide drastically. Since the formation of the transition layer is dominated by diffusion of oxygen near the interface, the existence of point defects such as vacancies and interstitials should affect the diffusion of oxygen and thus, the formation of the interfacial layer.

Stability of interfaces between the high-k gate oxide and a silicon substrate, and/or between the high-k oxide and gate metal is, therefore, one of the crucial issues for the reliability of the MOS structure. In addition to this interfacial reliability issue, quantum chemical molecular dynamics analysis showed that the quality of the high-k oxide film was deteriorated seriously by point defects in the film, such as oxygen vacancy, interstitial oxygen and carbon because of the formation of the impurity states in the band gap of the film. [6]-[8] In particular, unexpected drastic decrease of the effective band gap of a hafnium dioxide thin film was caused by interstitial carbon atoms which remain in the film in large quantities after the film deposition process using organic gas sources. Though post oxidation annealing was effective for recovering the defects-induced damages of the film, surplus oxygen atoms which remained after the oxidation of the film caused the growth of the interfacial metal oxide during the deposition of gate metal and thus, degraded the quality of the stacked structure.

In this study, the degradation mechanism of the interface integrity between a hafnium dioxide thin film and a gate electrode thin film was investigated by using quantum chemical molecular dynamics. The estimated changes of the interface structure were confirmed by experiments using synchrotron radiation photoemission spectroscopy.

ANALYTICAL MODEL

Quantum chemical molecular dynamics simulations were applied to the analysis of the HfO_2/W stacked structure using the colors code [9]. Since an extend Hückel approximation is used in this program to solve the electronic state as shown in the equation (1), we have to optimize the empirical parameters used in Hamiltonian.

orbital energy — repulsion interaction energy

$$E=\sum_{i=1}^{N}\frac{1}{2}m_i v_i^{\,2}+\sum_{k=1}^{OCC}\varepsilon_k+\sum_{i=1}^{N}\sum_{j>i}^{N}\frac{Z_i Z_j e^2}{r_{ij}}+\sum_{i=1}^{N}\sum_{j>i}^{N}E_{repuls}(r_{ij})$$

kinetic energy — Coulomb interaction energy

Repulsion term: $E_{repuls}(r_{ij})=f_0 b_{ij}\exp\left(\frac{a_{ij}-r_{ij}}{b_{ij}}\right)$ (1)

In this study, All atomic parameters were determined on the basis of density functional theory (DFT) calculations and considering the experimental results to satisfy the measured properties such as the geometry, binding energies, atomic charges, density of states of Hf, W, HfO_2, WO_3 bulk structures and so on. DFT calculations were performed by using CASTEP code. We employed the generalized gradient approximation (GGA) of Perdew et al. [10] for the exchange correlation functional. In this study, we analyzed the structural and

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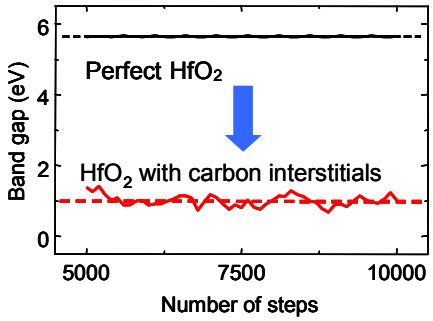

FIGURE 1 OXYGEN VACANCY-INDUCED DECREASE OF THE LOCAL BAND GAP OF HAFNIUM OXIDE. AN OXYGEN VACANCY GENERATES A DONOR STATE IN THE BAND GAP OF THE HAFNIUM OXIDE, AND THUS DECREASES THE LOCAL BAND GAP AROUND THE VACANCY SITE.

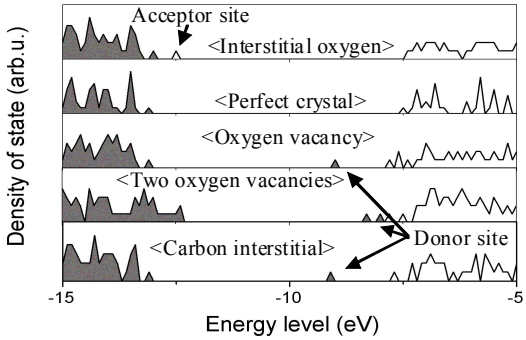

FIGURE 2. POINT DEFECTS-INDUCED IMPURITY STATES IN THE BAND GAP OF HAFNIUM OXIDE.

electronic properties of W/HfO_2 with oxygen vacancies and carbon interstitials. The magnitude of the band gap is a dominant factor that determines the dielectric properties of the gate oxide film. However, the magnitude of the band gap of HfO_2 and WO_3 calculated by a regular DFT method is much smaller than that of the experimental results.

On the other hand, the magnitude of the band gap of HfO_2 and WO_3 determined by the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) calculated by our method was 5.7 eV and 2.7 eV, respectively. These values agreed well with the reported experimental results. We modeled the structure of HfO_{2-x}, which is HfO_2 with oxygen vacancies, by eliminating oxygen atoms from the unit cell. For the unit cell of HfO_2 with carbon interstitial model, a few carbon atoms were introduced in HfO_2 structure. The molecular dynamics simulations were performed for 10,000 steps with a time step of 0.5 $\times 10^{-15}$ seconds at several temperatures.

The magnitude of the band gap is a dominant factor that determines the dielectric properties of the gate oxide film. The effect of various point defects on the band gap of the hafnium oxide was analyzed by calculating the change of the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) caused by the introduction of the point defects.

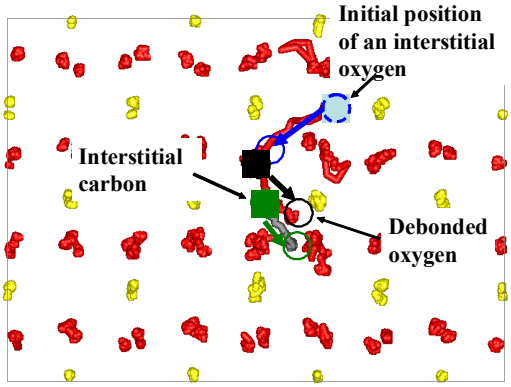

FIGURE 3 TRAJECTORIES OF HAFNIUM, OXYGEN AND CARBON ATOMS IN $HfO_{2+X}C_Y$. A CARBON INTERSTITIAL EASILY GENERATES AN OXYGEN VACANCY. AN OXYGEN-INTERSTITIAL, IF IT EXISTS NEAR THE VACANCY SITE, OCCUPIES THE DEFECTED SITE, AND THUS, RECOVERS IT.

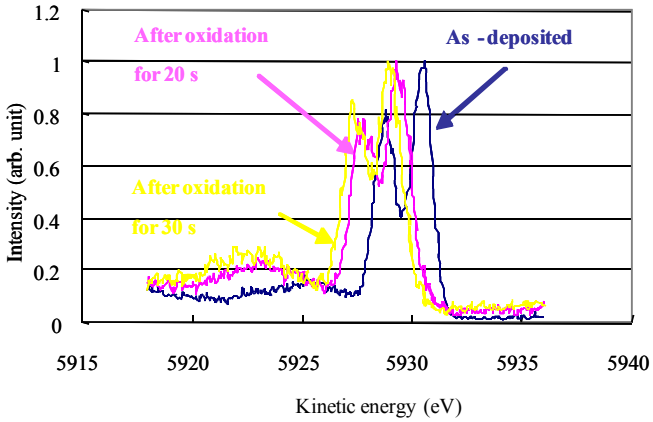

FIGURE 4 CHANGE OF THE HF-4F SPECTRUM DUE TO THE CHANGE OF THE COMPOSITION OF THE HAFNIUM OXIDE BEFORE THE DEPOSITION OF GATE ELECTRODE.

ANALYTICAL RESULTS

Quantum chemical molecular dynamics analysis showed that the quality of the high-k oxide film was deteriorated seriously by point defects in the film, such as oxygen vacancies, oxygen and carbon interstitials because of the formation of the impurity states in the band gap of the film. Carbon interstitials that is often introduced by atomic layer deposition (ALD) or metal-organic chemical vapor deposition (MOCVD) process using an organic gas source. Unexpected drastic decrease of the local effective band gap of a hafnium dioxide thin film from 5.7 eV to about 1 eV was caused by interstitial carbon atoms which remain in the film in large quantities after the film deposition process using the organic gas sources as shown in Fig. 1. This is because that the interstitial carbon atoms interact with hafnium atoms, i.e., deoxidize the hafnium oxide, and thus, easily make oxygen vacancies.

An extra "HOMO" peak appears in the band gap due to the oxygen vacancy and thus, the donor states are generated in the band gap of hafnium dioxide as shown in Fig. 2. The defect-induced site is formed by the dangling 5d orbital of a hafnium atom. In addition,

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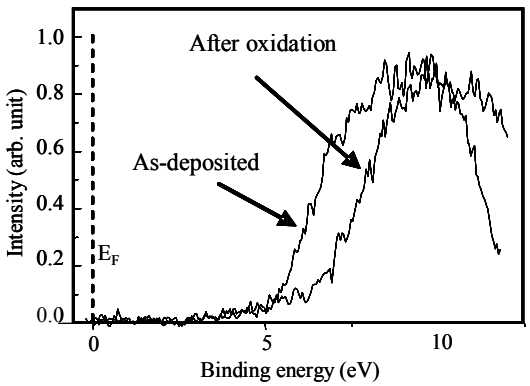


FIGURE 5 SYNCHROTRON-RADIATION PHOTOEMISSION SPECTRA OF THE $HfO_{2-X}C_Y$ FILMS NEAR THE EDGE OF THE FERMI LEVEL. THE PEAK SHIFTS CLEARLY OCCURS DEPENDING ON THE CHANGE OF DENSITIES OF OXYGEN VACANCIES AND CARBON INTERSTITIALS. DECREASE OF THESE DEFECTS INCREASES THE WIDTH OF THE BAND GAP OF THE FILMS AND THUS, IMPROVES THE QUALITY OF THE FILM.

some interstitial carbons substitute the debonded site. The substituting carbon atoms can form stable bonds with hafnium atoms in HfO2-xCx structure and thus, the electronic structure around the carbon atom seems to be similar to that of the hafnium carbide. The strong interactions between carbon and hafnium atoms give rise to a serious shrinkage of local band gap of the hafnium dioxide because hafnium carbide has a good electric conductivity. Post-oxidation annealing is effective for minimizing these defect sites. The excessive oxygen atoms introduced into the film by oxidation oxidize carbon and substitute the defect sites as shown in Fig. 2. Thus, the post-oxidation annealing can improve the quality of the oxide.

The effect of the post-oxidation annealing on the improvement of the quality of the annealed oxide was validated by synchrotron radiation photoemission spectroscopy as shown in Fig. 4. The binding energy of Hf-4f clearly shifted to the lower kinetic energy side, i.e., higher binding energy side, when the defect density was low. This chemical shift indicates that the atomic bonding condition became unstable when the defect density was high. In addition, the change of the peak position of the sub peak that appeared at the kinetic energy between 5920 eV and 5925 eV indicates the change of the band gap structure of the films. The width of the peaks of the film with low density of the defects was wider than that with high density of the defects. This increase of the peak width may indicate the increase of residual strain in the film. Similar shift and change were observed in O-1s peak of all the oxidized films.

Actually, the increase of the band gap of the $HfO_{2-x}C_y$ film by post-oxidation annealing was also validated by synchrotron radiation photoemission spectroscopy. The reduction of oxygen vacancies and carbon interstitials in the $HfO_{2-x}C_y$ films increased the band gap of the films significantly as shown in Fig. 5. The change of the band width was about 1 eV. This result clearly shows that the increase of point defects such as oxygen vacancies and carbon interstitials decreases the band gap of hafnium dioxide films and deteriorates the film quality. For example, the gate leakage current of a MOS transistor after the post-oxidation annealing was found to decrease drastically. Since the effective relative permittivity is a function of band gap of oxide, this change of the band gap causes the change of the effective capacitance of a MOS structure. These changes caused by the shift of the band gap should affect the electronic performance of a MOS transistor significantly. One of the reasons for the fluctuation of the electronic performance of MOS transistors with high-k dielec

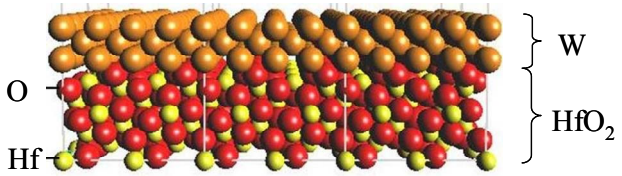
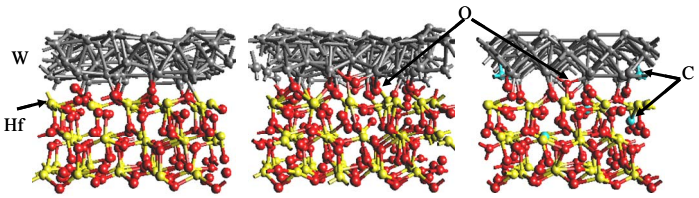


FIGURE 6. BASIC MD SIMULATION MODEL OF A HIGH-K GATE OXIDE WITH GATE METAL. OXYGEN AND CARBON INTERSTITIALS ARE INTRODUCED INTO THIS MODEL TO ANALYZE THE EFFECT OF THESE POINT DEFECTS ON THE ELECTRONIC BAND STRUCTURES OF HAFNIUM OXIDE AND THE STABILITY OF THE INTERFACE BETWEEN THE OXIDE AND A TUNGSTEN GATE ELECTRODE.



(a) W on HfO_2 (b) W on $HfO_{2.13}$ (c) W on $HfO_{2.04}C_{0.1}$

FIGURE 7. EXAMPLES OF THE ESTIMATED CHANGE OF THE INTERFACIAL STRUCTURES BETWEEN THE HAFNIUM OXIDE AND TUNGSTEN GATE DEPENDING ON THE COMPOSITION OF THE OXIDE BEFORE THE DEPOSITION OF THE GATE. TUNGSTEN OXIDE OR TUNGSTEN CARBIDE WAS GROWN PARTIALLY NEAR THE INTERFACE WHEN OXYGEN AND CARBON INTERSTITIALS REMAINED IN THE HAFNIUM OXIDE BEFORE THE DEPOSITION OF THE TUNGSTEN GATE.

trics can be attributed to the fluctuation of the composition of the oxide such due to carbon interstitials and oxygen vacancies remained in the oxide.

Next, the effect of the remained point defects such as oxygen vacancies, oxygen interstitials, and carbon interstitials in the hafnium oxide after the post oxidation annealing on the integrity of the interface between the oxide film and the deposited metal was analyzed by quantum chemical molecular dynamics. In this study, the structural and electronic properties of monoclinic HfO_2 with oxygen and carbon interstitials were analyzed by using a three-dimensional atomic model as shown in Fig. 6. The total number of atoms in this mode was 204. Some surplus oxygen or carbon atoms were also introduced in this model.

Figure 7 shows the examples of the estimated results of the effect of the remained oxygen and carbon interstitials in the hafnium oxide on the interfacial structure between the oxide and tungsten. When there were no interstitials in the oxide, the interface was clear and no oxygen atoms diffused into the deposited tungsten gate. Thus, an ideal interface structure can be achieved if the perfect hafnium dioxide is prepared before deposition of the gate metal. On the other hand, some oxygen atoms diffused into the tungsten film and thus, tungsten oxide is grown partially around the interface, when the excess oxygen interstitials remained in the hafnium oxide film ($HfO_{2.13}$) before the deposition of the tungsten film. Though post-oxidation annealing is effective for improving the electronic quality of the hafnium oxide with oxygen vacancies, heavy oxidation should deteriorate the interfacial integrity of MOS structures.

In addition, the remained carbon interstitials also diffused out from the hafnium oxide and diffused into the tungsten film and formed tungsten carbide around the interface ($HfO_{2.04}C_{0.1}$). This formation of carbide also changes the electronic band structure between

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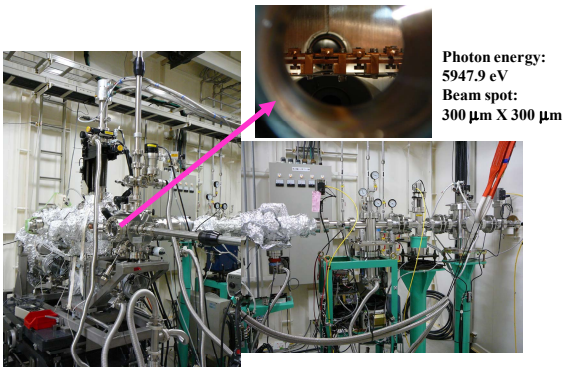

FIGURE 8 OUTLOOK OF SYNCHROTRON PHOTOEMISSION SPECTROSCOPY

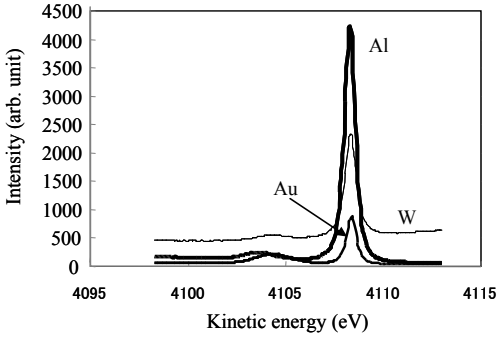

FIGURE 10. CHANGE OF THE SI-1S SPECTRUM DUE TO THE CHANGE OF THE MATERIAL OF A GATE ELECTRODE.

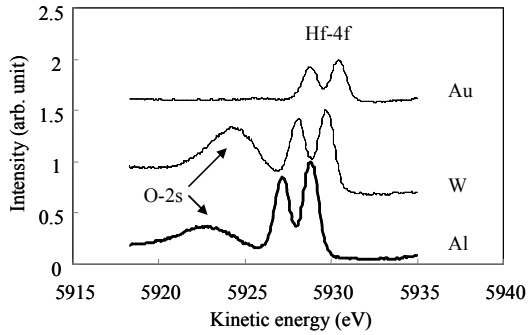

FIGURE 9. CHANGE OF THE HF-4F SPECTRUM DUE TO THE CHANGE OF THE MATERIAL OF A GATE ELECTRODE. CLEAR PEAK OF O-2S APPEARED WHEN THE GATE MATERIAL WAS TUNGSTEN AND ALUMINUM, WHILE NO O-2S PEAK APPEARED WHEN THE GATE MATERIAL WAS GOLD.

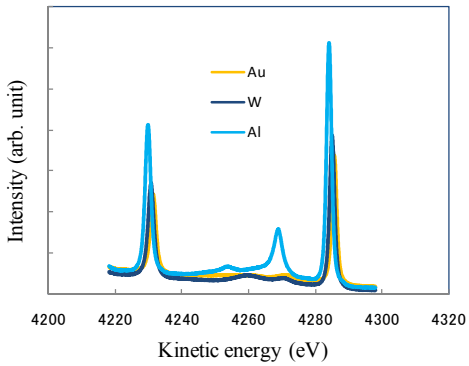

FIGURE 11. CHANGE OF THE HF-3D SPECTRUM DUE TO THE CHANGE OF THE MATERIAL OF A GATE ELECTRODE.

the oxide and metal. Thus, both the composition of the hafnium oxide film and the interfacial structure between the oxide and the deposited tungsten film varied significantly depending on the composition of the hafnium oxide before the deposition of the tungsten film. Therefore, the composition control of the hafnium oxide film before the deposition of gate metal is very important to assure the electronic quality of the stacked structure.

When the material of the metal electrode was changed from tungsten to gold, the interface structure was found to become stable regardless of the composition of the hafnium oxide. No change of the electronic band structure was estimated. Thus, interface structure between the oxide and metal during the quality evaluation of this oxide should be exactly the same as that of actual transistors.

PHOTOEMISSION SPECTROSCOPY AND RESULTS

The estimated point defects-induced change of the interfacial structure between the $HfO_{2+x}C_y$ film and the gate electrode was validated by synchrotron-radiation photoemission spectroscopy shown in Fig. 8. A high-energy excitation source (5947.3 eV) enabled to analyze the chemical shift of the component elements in the 4-nm thick $HfO_{2-x}C_y$ films with metal gate of 4-nm thick tungsten, aluminum, and gold. Hafnium dioxide thin films of 4-nm thick were deposited by ALD. These films contained large density of carbon interstitials and oxygen vacancies. Post oxidation annealing was performed after the film deposition. The oxidation time was varied to change the concentration of the remained surplus oxygen before the deposition of a metal gate. The spectra of O-1s, C-1s, and Hf-4f, for example, were compared one after another to evaluate the defect density in the films. Detection angle of the photoemission spectroscopy was fixed at 88 deg.

Figure 9 shows the measured change of the spectrum of Hf-4fcaused by the change of material of the gate electrode deposited on $HfO_{2+x}C_y$. It was found that the peak of O-2s appeared clearly when the gate electrode material was tungsten or aluminum. On the other hand, no clear peak of the O-2s was observed when the gate electrode material was gold. This result indicated that both aluminum and tungsten gates were oxidized partially. This oxidation can be attributed to the excess oxygen in the hafnium oxide before the deposition of the electrodes. In addition, the peak positions of Hf-4f varied substantially depending on the gate electrode material. This peak shift indicates that the quality of the hafnium dioxide changed significantly depending on the gate electrode material. No substantial change was observed in the spectrum of Si-1s regardless of the gate electrode material as shown in Fig. 10. Thus, this spectrum change of Hf-4f mainly occurred near the interface between the hafnium oxide and the gate electrode. Detection angle of the photoemission spectroscopy was changed from 88 deg to 30 deg to confirm that the O-2s peak appeared only around the interface. The intensity of the O-2s peak increased drastically after the change of this detection angle. This result clearly indicated that the there is a strong gradient of oxygen and the concentration of oxygen around the interface was higher than that in the oxide. Thus, it can be concluded that interstitial oxy

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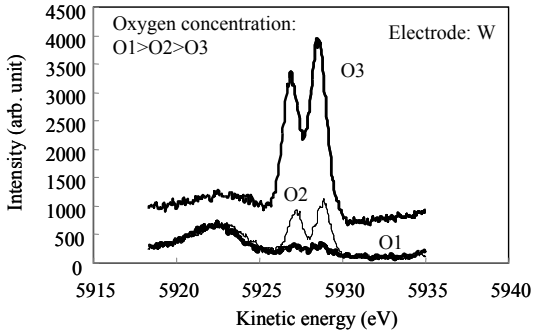

FIGURE 12. CHANGE OF THE HF-4F SPECTRUM DUE TO THE CHANGE OF THE COMPOSITION OF THE HAFNIUM OXIDE BEFORE THE DEPOSITION OF A TUNGSTEN FILM. THE CONCENTRATION OF OXYGEN INTERSTITIAL WAS VARIED BY CONTROLLING THE POST OXIDATION TIME. THE PEAK HEIGHT OF THE O-2S DECREASED DRASTICALLY WITH THE DECREASE OF THE CONCENTRATION OF SURPLUS OXYGEN INTERSTITIALS.

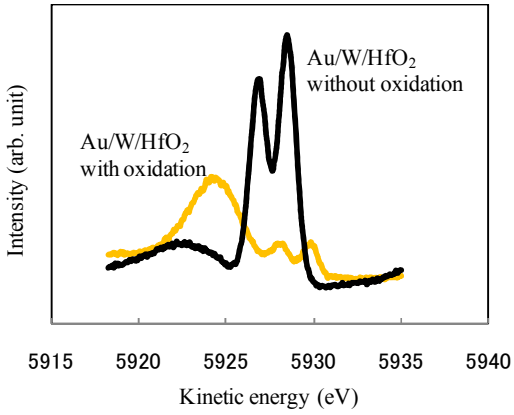

FIGURE 13. CHANGE OF THE HF-4F SPECTRUM DUE TO THE CHANGE OF THE COMPOSITION OF THE HAFNIUM OXIDE BEFORE THE DEPOSITION OF A STACKED GATE STRUCTURE OF GOLD AND TUNGSTEN.

gen atoms diffused out from the oxide and it diffused into the gate metal and thus, oxidized the gate metal partially.

Figure 11 shows change of the spectrum of Hf-3d by changing the material of gate electrode. Two main peaks exist at almost the same position of about 4227 eV and 4283 eV regardless of the electrode material. The small peak between these peaks was observed when aluminum was deposited on the oxide. This peak corresponds to aluminum oxide. When gold was deposited on the oxide, no change of these peaks was observed between before and after the deposition of the gold electrode. Thus, the interface structure around the hafnium oxide and metal electrode is a strong function of the material of the gate electrode.

Since the surface oxidation of the gate electrode material may have been the main reason for the spectrum change, the Hf-4f spectrum was measured by changing the concentration of the remained oxygen interstitials in the hafnium dioxide before the deposition of the tungsten gate electrode as shown in Fig. 12. The concentration of the remained excessive oxygen interstitials was changed by controlling the duration time of the post oxidation annealing. This figure clearly shows that the peak height of the O-2s decreases drastically when the oxidation time was decreased and thus, the concentration of the remained oxygen interstitials was decreased. Therefore, the observed gate electrode material dependence of the Hf-4f peak shown in Fig. 9 was mainly attributed to the diffusion of the remained excessive oxygen in the hafnium dioxide film into the deposited tungsten gate electrode. The formation of tungsten oxide or aluminum oxide was also confirmed by the measurement of the spectra of W-4f, and Al-1s.

Since the formation of metal-oxide and metal-carbide increases the effective thickness of the oxide in a MOS structure, such contamination of the metal gate should deteriorate the electronic performance and reliability of MOS transistors. From this point of view, the contamination of high-k dioxides that is caused by the remained carbon interstitials and oxygen vacancies should be eliminated before the deposition of gate metal. As it was mentioned before, post-oxidation annealing is an effective way for decreasing these defects. However, since the excessive oxygen interstitials remained in the oxide after the post-oxidation annealing also degrades the quality of MOS transistors, the compositional control of the oxide after the annealing is very important to improve both the electronic performance and reliability of MOS transistors with high-k gate oxide.

In order to confirm the importance of the interface structure between the hafnium oxide and metal gate, a stacked gate structure which consisted of gold and tungsten was deposited on the hafnium oxide (Au/W/Oxide) as shown in Fig. 13. Before the deposition, the concentration of excess oxygen was varied by controlling the duration time of the post-oxidation after the deposition of the oxide. Even if gold was deposited on the top surface of the stacked gate, clear O-2s peal appeared when the concentration of the remained oxygen interstitials increased. This result indicated that the bottom tungsten was oxidized by the excess oxygen in the oxide which was introduced into the oxide by post-oxidation. Thus, the interface structure between the oxide and electrode is very important to assure the integrity of the interface.

Therefore, it is very important to minimize the concentration of both the remained oxygen and carbon interstitials in the hafnium oxide before the deposition of a gate electrode because both oxygen interstitials and carbon interstitials diffuse out from the oxide and thus, oxidize the gate electrode material. In order to protect the oxidation of the gate electrode material, the introduction of a diffusion barrier layer between the hafnium oxide and the gate electrode material is indispensable for assuring the high quality of the stacked structure. Gold is one of the effective candidates for the diffusion barrier material.

CONCLUSION

Point defects such as oxygen vacancies and interstitials, and carbon interstitials deteriorate the electronic quality of the hafnium dioxide deposited by using an organic gas source. This is because that the impurity sites such as donor sites and acceptor sites are appeared in the electronic band structure of the oxide. Therefore, post-oxidation annealing is effective for minimizing these defect sites and thus, improves the quality of the oxide.

The interfacial structure between the hafnium dioxide and gate metal is also deteriorated by the formation of metal-oxide or carbide around the interface. The analytical results estimated by quantum chemical molecular dynamics were validated by synchrotron radiation photoemission spectroscopy. It is very important, therefore, that the minimization of point defects in the hafnium dioxide films before the deposition of the gate electrode material. Besides, the introduction of a diffusion barrier layer between them is indispensable for

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improving the electronic performance and reliability of the stacked structure.

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